Amendments To The Claims

1. (*Currently Amended*) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function;

(d) deconvoluting said M compounds into their associated reagent building blocks;

(e) generating ~~said~~ a focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting from said at least one compound enumerated from said focused library at least one K compound based on said at least one fitness function; and

(h) ~~synthesizing~~ outputting a list of said at least one K compound.

2. (*Canceled*)

7. (*Previously Presented*) The method of claim 1, wherein the at least one fitness function in step (c) is selected from similarity, diversity, and presence or absence at least one characteristic.

8. (*Currently Amended*) The method of claim 7, wherein said focused library of at least one compound includes a plurality of compounds~~, wherein step (g) further comprises: selecting at least one K compound from said focused library of compounds based on said fitness function and outputting a list of said at least one K compound~~.

10. (*Previously Presented*) The method of claim 8, wherein step (c) comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said initial sub-set of M compounds based on said fitness function; and

(iii) refining said initial sub-set of M compounds based on said fitness function, thereby selecting said M compounds.

11. (*Previously Presented*) The method of claim 10, wherein step (g) comprises:

(i) selecting an initial sub-set of at least one K compound from said focused library of compounds;

(ii) evaluating said initial sub-set of at least one K compounds based on said fitness function; and

(iii) refining said initial sub-set of at least one K compound based on the fitness function, thereby selecting said at least one K compound.

12. (*Previously Presented*) The method of claim 11, wherein said fitness function is related to diversity of a collection of compounds, and wherein step (c)(ii) comprises evaluating a diversity of said initial sub-set of M compounds, and wherein step (c)(iii) comprises refining said initial sub-set of M compounds to increase said diversity of said M compounds

13. (*Previously Presented*) The method of claim 12, wherein said initial sub-set of at least one K compound comprises a plurality of K compounds wherein step (g)(ii) comprises evaluating the diversity of said initial sub-set of K compounds, and wherein step (g)(iii) comprises refining said initial sub-set of K compounds to increase the diversity of said K compounds.

14. (*Previously Presented*) The method of claim 8, wherein step (c) comprises:

(i) characterizing said N enumerated compounds;

(ii) evaluating said characterized N enumerated compounds based on said fitness function;

(iii) ranking said characterized N enumerated compounds based on said evaluation; and

(iv) selecting said M compounds based on said ranking.

15. (*Previously Presented*) The method of claim 14, wherein said focused library of at least one compound comprises a plurality of compounds, wherein step (g) comprises:

(i) characterizing said compound of said focused library of compounds;

(ii) evaluating said characterized compound of said focused library of compounds based on said fitness function;

(iii) ranking said characterized compounds of said focused library of compounds based on said evaluation; and

(iv) selecting said K compounds based on said ranking.

16. (*Previously Presented*) The method of claim 15, wherein step (c)(i) comprises characterizing said N enumerated compounds using a set of molecular descriptors.

17. (*Previously Presented*) The method of claim 16, wherein step (g)(i) comprises characterizing compounds of said enumerated focused library of compounds using said set of molecular descriptors.

18. (*Previously Presented*) The method of claim 15, wherein said fitness function is related to a similarity to one or more query structures, and wherein step (c)(ii) comprises evaluating similarity between said N enumerated compounds and said one or more query structures.

19. (*Previously Presented*) The method of claim 18, wherein at least one of the following similarity measures is used in step (c)(ii) for evaluating similarity between each compounds and said one or more query structures:

(1) similarity in number of atoms, bonds and rings of the same types;

(2) similarity in shape and surface characteristics;

(3) similarity in electron density distribution;

(4) similarity based on common substructure;

(5) similarity based on the presence and orientation of pharmacophoric groups;

(6) similarity in binding affinity; and

(7) similarity in degree of conformational overlap with a know receptor binder.

20. (*Previously Presented*) The method of claim 18, wherein step (g)(ii) comprises evaluating similarity between compounds of said enumerated focused library of compounds and said one or more query structures, and wherein the same similarity measure is used for evaluating similarity in step (c)(ii) and step (g)(ii).

21. (*Previously Presented*) The method of claim 14, wherein said fitness function is related to at least one desired characteristic, and wherein step

(c)(ii) comprises evaluating N enumerated compounds to determine an extent to which the N enumerated compounds possess the at least one desired characteristic.

22. (*Previously Presented*) The method of claim 21, wherein the at least one desired characteristic comprises at least one of the following:

(1) a desired physical property;

(2) a desired chemical property;

(3) a desired functional property; and

(4) a desired bioactive property.

23. (*Currently Amended*) A computer based system for analyzing a non-enumerated virtual library, comprising:

means for randomly selecting a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds;

means for enumerating said set of N compounds;

means for selecting M compounds of said set of N enumerated compounds based on a fitness function;

means for deconvoluting said M compounds into their associated <u>reagent</u> building blocks;

means for generating a ~~said~~ focused library of compounds based on said building blocks;

means for enumerating a plurality of said compounds of said focused library of compounds; ~~and~~

means for selecting at least one K compound of said enumerated compounds of said focused library based on the fitness function,

~~wherein~~ means for outputting to a user said at least one selected K compound ~~is~~ to be synthesized.

24. (*Canceled*)

25. (*Canceled*)

26. (*Canceled*)

31. (*Canceled*)

32. (*Canceled*)

34. (*Canceled*)

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40. (*Canceled*)

41. (*Canceled*)

42. (*Canceled*)

43. (*Canceled*)

44. (*Canceled*)

45. (*Canceled*)

46. (*Canceled*)

47. (*Canceled*)

48. (*Canceled*)